

A

ZINC15 kinase subset
available now, anodyne

10883

intersection with eMolecules library

1204

availability through eMolecules

Tier1, 100 mg, powder

292

predicted pK_a filter

Epik Sequential pK_a

- at least one pK_a value in range 3-11
- pK_a values at least 1 pK_a unit apart

180

predicted logP filter

-1 ≤ OpenEye XlogP ≤ 6

178

FRAGMENT-LIKE

DRUG-LIKE

150 ≤ mw < 350

molecular weight filter

350 < mw ≤ 500

126

47

price listed and 100 mg available

111

40

filter out molecules with experimental logP

91

15

compound selection rules

1. Include at least one molecule for each kinase inhibitor ring fragment
2. Limit the number of frequently appearing rings to at most one
3. Target broad and uniform sampling of logP dynamic range
4. Prioritize cheaper molecules

25 (17)

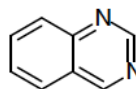
10 (7)

B

Heterocycles found frequently in FDA approved kinase inhibitors



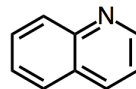
pyridine



quinazoline



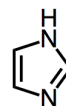
pyrimidine



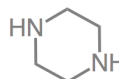
quinoline



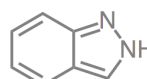
pyrazole



imidazole



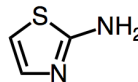
piperazine



indazole

C

Heterocycles overrepresented in fragment libraries



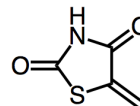
aminothiazole



thiophene



1,3,4-thiadiazole



5-methylenethiazolidine-2,4-dione